Simulation of LNAPL flow in the vadose zone using a single phase flow equation

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Abstract

Multiphase flow simulators are often used for environmental investigations of LNAPL migration in the vadose zone and on the water table of unconfined aquifer systems. Their immense computational burden, however, is prohibitive for their application to large complex three-dimensional systems. Simplifying assumptions that are often made to enable required analyses include use of coarse gridding, reduced (one- or two-dimensional) dimensionality, simplified geometries, small areal extents, smoothened parameterization and limited evaluations rendering the results unusable or unreliable. Many investigations of environmental LNAPL concerns may not warrant solution to the multiphase system of equations and assumptions for reducing the equation set may be more practical and applicable, as discussed here. Simplification of the constitutive relationships further allows solution to this class of environmental analysis problems, by using commercially available vadose zone simulation software with minimal modifications. Justification and impact of assumptions and simplifications of reducing the equations and the constitutive relationships are discussed and example problems are provided to demonstrate accuracy and application of the simplified approach.

Introduction

LNAPLs (light non-aqueous phase liquids) are chemical compounds or mixtures of compounds that do not fully mix with water and have a density that is less than that of water. Spills and releases of LNAPLs on soil, or leakage from underground storage tanks and pipelines cause soil and groundwater contamination, which pose environmental concerns regarding their migration and fate. Multiphase flow simulators are often used for environmental investigations of LNAPL migration in the vadose zone and on the water table of unconfined aquifer systems. The US Environmental Protection Agency's National Service Center for Environmental Publications (NSCEP) lists NAPL Simulator (Guarnaccia et al, 1997) and UTCHEM (Pope et al, 1999) among their LNAPL simulation programs. Other multiphase flow simulators have also been developed and applied towards environmental evaluations of LNAPL migration in the subsurface (Falta et al, 1995; White and Oostrom, 2006). These numerical simulators discretize the subsurface into computational cells and solve the transient equations for the flow of air, LNAPL and water at each time-step, to determine the state of LNAPL and its migration in the unsaturated soil and at the water table. These multiphase simulators tend to be computationally intensive because they solve for multiple equations per computational cell and because of the extremely non-linear nature of the interactions between the phases and of the various constitutive relationships. Simplifying assumptions that are often made to enable required analyses include use of coarse gridding, reduced (one- or two-dimensional) dimensionality, simplified geometries and small areal extents to reduce the size of the problem. Furthermore, parameter values may be smoothened to relieve nonlinearity and limited evaluations can be conducted because of convergence issues rendering the results unusable or unreliable.

The hypothesis of the current work is that only one (LNAPL phase) equation needs to be solved for evaluating LNAPL flow in the vadose zone and along the water table. This is significant because it enables simulation of larger domains with finer grids, fully three-dimensional representations, and structural complexity that may be difficult or impossible to represent and solve at a complex contaminated site, with a multiphase flow model. First, the approach would significantly alleviate computational burden of the multiphase flow equations which are extremely hard to solve and computationally intensive and, depending on code used, can often fail even for very simple conditions. Also, reducing the number of equations further reduces the parameterization burden because the parameters and constitutive relations are now only needed for the LNAPL phase.

In addition to reducing the number of equations solved for evaluating LNAPL migration, the three-phase constitutive relationships may also be simplified to standard two-phase moisture retention and relative permeability functions by approximating a transformed pore space for the LNAPL flow simulations. Thus, the equations are same as the popular Richards Equation framework (Richards, 1931) used for solving variably saturated flow of water in the subsurface. Consequently, the formulation is readily adaptable to open source, public domain codes such as MODFLOW-USG enhancements available in USG-Transport (Panday et al, 2013, Panday, 2018), or HYDRUS (Šimùnek et al, 2008) which solve the Richards Equation. Finally, the impact of the hypotheses are tested by comparing results of this formulation to multiphase simulations of various examples using the UTCHEM model cited by NSCEP.

Approach and Impact

The proposed approach is to reduce governing multiphase flow equations using appropriate approximations to simplify and speed-up computations. The approach then further modifies the three-phase constitutive relationships into standard two-phase functions that are readily available in unsaturated zone simulation software.

The first assumption for reducing the governing equations, is that air phase instantly equilibrates to the movement of liquids within the subsurface. This assumption is reasonable for LNAPL flow in the unsaturated zone, because air in the unsaturated zone rapidly equilibrates with atmospheric conditions due to its significantly higher permeability than that of the liquids. In fact, this is the exact same assumption made by solving the Richards Equation for variably saturated water flow, and is well established for this purpose. In addition, the air flow dynamics are unimportant for many LNAPL migration investigations. Both these conditions may be significant for a petroleum reservoir but are not of consequence in evaluating environmental LNAPL migration in the vadose zone. Therefore, the air phase flow equation can be reduced with little potential impact.

The second assumption for reducing the governing equations, is that the state of water remains unchanged and that the flow dynamics and redistribution of water can be neglected. This is also reasonable in many situations, especially when steady or no recharge of water is considered during evaluations. There would be little if any impact above the capillary fringe where water is at residual saturation and therefore imbibition of LNAPL cannot further reduce the water saturation. Within the capillary fringe and at the water table, the pressure of invading LNAPL reduces water saturation and depresses the existing water table. However, if this change in water state is neglected and the water table is considered as a no-flow boundary to LNAPL, the lateral spreading of LNAPL will be larger, since LNAPL is not allowed to invade pore space occupied by existing water resulting in a higher mound with larger LNAPL head gradients. Thus, the potential impact of this assumption is to over-predict the lateral spreading of LNAPL within the capillary fringe and once it hits the water table. By evaluating the resulting LNAPL pressures and adjusting water saturations accordingly, the impact of this assumption can be further evaluated and bounded. Thus, the water phase flow equation can be reduced with potentially no impact to LNAPL migration in the vadose zone and bounded estimates of impacts to LNAPL migration within the capillary fringe and at the water table.

After reducing the air and water phase flow equation, only the LNAPL flow equation remains to be solved for LNAPL flow rates, pressure and saturation. Air is always at atmospheric pressure, and water pressures and saturations remain unchanged from their initial conditions and therefore the 3-phase constitutive relationships can be parameterized. However, a further simplification may be employed to the constitutive relationships to reduce them to 2-phase relationships used conventionally in unsaturated zone water flow models. This is because the water phase state is assumed to remain unchanged only the air-filled pore space is made available for LNAPL flow. The formulation for single phase LNAPL flow simulation for evaluation of environmental settings is presented next along with the simplifying assumptions to reduce the constitutive equations.

Equations for Multiphase LNAPL Flow

The governing equation for flow of the LNAPL phase is expressed as:

[EMBED Equation.DSMT4] (1)

Where [EMBED Equation.DSMT4] is the hydraulic head of the LNAPL phase defined as: [EMBED Equation.DSMT4], [EMBED Equation.DSMT4]is the pressure head of the LNAPL phase, and [EMBED Equation.DSMT4]is the elevation. [EMBED Equation.DSMT4]is the porosity, [EMBED Equation.DSMT4]is the saturation of LNAPL, [EMBED Equation.DSMT4] is time, [EMBED Equation.DSMT4] are the three principal coordinate directions, [EMBED Equation.DSMT4] is the relative permeability to LNAPL, [EMBED Equation.DSMT4] is the absolute permeability of soil, [EMBED Equation.DSMT4] is the density of LNAPL, [EMBED Equation.DSMT4] is the viscosity of LNAPL, and [EMBED Equation.DSMT4] is a LNAPL source flux rate (negative for sink). Similar governing equations are present for water and air phase flow in a 3-phase flow system, with the subscript "[

EMBED Equation.DSMT4]" replaced by "[EMBED Equation.DSMT4]" or "[EMBED Equation.DSMT4]" to denote water or air respectively.

The constitutive van Genuchten moisture content relations for a 3-phase water-wet system are expressed as:

[EMBED Equation.DSMT4] (2)

And

[EMBED Equation.DSMT4] (3)

Where [EMBED Equation.DSMT4] is the oil-water capillary pressure head, [EMBED Equation.DSMT4] is the air-oil capillary pressure head, [EMBED Equation.DSMT4], [EMBED Equation.DSMT4] , and [EMBED Equation.DSMT4], are the van Genuchten parameters for an air-water system, [EMBED Equation.DSMT4]and [EMBED Equation.DSMT4]are the effective saturations for water and total liquid defined as:

[EMBED Equation.DSMT4] (4)

And

[EMBED Equation.DSMT4] (5)

Where [EMBED Equation.DSMT4] is the water saturation, [EMBED Equation.DSMT4] is the residual water saturation, [EMBED Equation.DSMT4]is the residual LNAPL saturation, and [EMBED Equation.DSMT4] is the total liquid saturation. The effective water saturation in equation (4) accounts for the presence of residual LNAPL (Charbeneau, 2007). Thus, by definition,

[EMBED Equation.DSMT4] (6)

Also, the terms [EMBED Equation.DSMT4] and [EMBED Equation.DSMT4] are scaling factors depending on the interfacial tension ratios between air-water and the two indexed fluids. Thus,

[EMBED Equation.DSMT4] (7)

And

[EMBED Equation.DSMT4] (8)

These equations along with a relative permeability relation for each of the phases form the governing equations for 3-phase flow in a 3-phase system.

Reduction of Governing Equations and Constitutive Relationships

Neglecting the governing equations for flow of water and air in a multiphase system implies that air is at atmospheric conditions, and that water pressure and saturation remain unchanged from the initial conditions. That leaves the governing equation for flow of LNAPL (Equation 1) along with the constitutive relationships (equations 2-8).

Since air is at atmospheric pressure in the vadose zone and density of air is negligible in comparison to that of the liquids, [EMBED Equation.DSMT4] and the capillary head is equal to negative of the respective liquid pressure head in equations (2) and (3).

The initial state of water in the subsurface may be determined by solving the governing water flow equation (Richards Equation) using a capillary curve as per equation (2), for steady-state recharge conditions of water within the simulation domain. Often, a site is not pristine and the air-water interface is mediated through LNAPL so the capillary curve may be scaled using equation (7).

Once saturation of water is estimated, the LNAPL phase flow equation (1) computes a total liquid saturation with equations (3), (5) and (8) providing the relationship between the air-NAPL capillary head and the total liquid (LNAPL plus water) saturation. Therefore, a single-phase flow equation simulator such as HYDRUS or MODFLOW-USG can be used to solve the flow equation, with modification of the appropriate terms and inclusion of the total saturation constitutive relationships for three-phase systems. However, additional manipulation of the equations can be performed to further simplify the three-phase functions to standard two-phase constitutive relations that are already available in unsaturated zone flow simulators.

A redefinition of the pore space is considered as an additional step for evaluation of LNAPL flow in the vadose zone using two-phase constitutive relationships. This can be performed because the water phase state is already assumed fixed and unchanging, and therefore LNAPL displaces only air within the voids during imbibition or drainage. Consequently, a modified porosity can be defined for LNAPL flow within which the voids represent only LNAPL and air. Since water (including residual water saturation) is excluded from the modified pore space (i.e., incorporating water as part of the non-void space in the volume computations), the remaining total liquid is only LNAPL.

The modified porosity is derived as follows. By definition, for a three phase system,

[EMBED Equation.DSMT4] (9)

Where [EMBED Equation.DSMT4], [EMBED Equation.DSMT4], [EMBED Equation.DSMT4] and [EMBED Equation.DSMT4] are the water, LNAPL, air, and total volumes respectively. The modified porosity that excludes water volumes is defined as:

[EMBED Equation.DSMT4] (10)

Manipulating equations (9) and (10), the modified porosity is expressed in terms of the actual porosity and the initial (fixed) water saturation as

[EMBED Equation.DSMT4] (11)

With use of this modified porosity in equation (1), the flow of LNAPL may be solved assuming water state is unchanging. Within this modified void space, the total saturation in equation (3) represents the saturation of only LNAPL since[EMBED Equation.DSMT4] and [EMBED Equation.DSMT4] are zero in this modified void space that excludes water from its definition. Equation (6) also reduces to the standard two-phase effective saturation definition with [EMBED Equation.DSMT4] and [EMBED Equation.DSMT4] equal to zero. Thus, equations (3) and (6) are equivalent to the standard two-phase van Genuchten retention function. The standard two-phase Brooks-Corey moisture retention function could also similarly be equated by reducing its three-phase counterpart.

The relative permeability of NAPL in a 3-phase system is expressed by the van Genuchten function as:

[EMBED Equation.DSMT4] (12)

Expressing this equation for the modified void space (wherein [EMBED Equation.DSMT4] and [EMBED Equation.DSMT4] equal to zero) gives

[EMBED Equation.DSMT4] (13)

Equation (13) is the same as the relative permeability for water in Richards Equation with the subscript “n” replaced by “w”. A similar reduction occurs also for the Brooks-Corey relative permeability function.

To incorporate a residual LNAPL saturation in equation (13), the effective LNAPL saturation of equation (6) is redefined in the modified porosity space as per equation (14) below. This effective LNAPL saturation is applied only to the relative permeability term and not to the LNAPL retention curve of equation (3). This causes LNAPL to build-up above its residual saturation before it flows any further during the LNAPL imbibition stage, and residual saturation of LNAPL to be left behind during the drainage stage.

[EMBED Equation.DSMT4] (14)

Where [EMBED Equation.DSMT4]is the residual saturation of LNAPL, and the subscript “m” further indicates that the LNAPL saturations are applied to the modified porosity, whereas it is the LNAPL volumetric content that is conserved. Therefore, the LNAPL saturation within the actual porosity of the medium can be obtained as

[EMBED Equation.DSMT4] (15)

where the second equality results from the use of equation (11). A similar relationship exists for the residual NAPL saturations, which is written in a rearranged form as

[EMBED Equation.DSMT4] (16)

The advantage of modifying the void space definition is that the LNAPL saturation and relative permeability can be computed by the standard two-phase constitutive relationships which are scaled representations of the van Genuchten/Brooks Corey equations for flow of water. Therefore the LNAPL flow equation can be solved by any code that solves the Richards Equation with the van Genuchten/Brooks Corey functions, with only one minor modification, that S_r be used only for relative permeability and not for the moisture retention when solving for LNAPL flow. As an aside, it could be argued that this residual condition (on the relative permeability and not on moisture retention) should be applied to the water flow solutions as well, to allow for evaporation or other sinks to reduce water saturations below residual levels for flow.

Subsurface water phase flow equations are typically expressed in terms of a water hydraulic conductivity instead of a combination of soil and fluid dependent parameters, and thus

[EMBED Equation.DSMT4] (17)

In that case, the hydraulic conductivity for water should be appropriately scaled as per equation (18) below, to give a NAPL flow conductivity term.

[EMBED Equation.DSMT4] (18)

Simulation Approach using a Richards Equation Solver

The approach to a NAPL simulation in the vadose zone using a standard Richards Equation solver is as follows:

1. Characterize the saturation state of water in the system. Water saturation can be computed by solving the Richards Equation for flow of water in the domain. Conditions of zero recharge are typically assumed but spatially variable recharge of water can be accommodated by any solution scheme, and the code can be run long enough to reach a steady-state condition. The water capillary curve is expressed by equation (2) with equation (7) providing the scaling term to express the presence of NAPL in the system.
2. Set up the Richards Equation Solver for simulating NAPL flow. Alter the van Genuchten moisture retention curve to optionally use a zero residual saturation. The relative permeability curve is unaltered to allow LNAPL flow only if saturations are above residual.
3. Setup domain for NAPL flow simulation. Using the same grid as for the water flow simulation of step 1, provide no-flow conditions at and below the water table (i.e., in all cells where $S_w = 1$ as simulated in step 1).

4. Using the water saturation from step 1, modify the porosity of the domain as per equation (11) to account for the space occupied by water.
5. Modify the hydraulic conductivity of the domain as per equation (18) to convert the saturated hydraulic conductivity to a flow conductivity value for LNAPL.
6. Modify the van Genuchten alpha parameter of the soils as per equation (8) to represent air-NAPL capillarity via scaling.
7. Modify the residual LNAPL saturation value as per equation (16) to represent NAPL contents within the modified porosity field of equation (11).
8. Apply the LNAPL source boundary conditions at the source location as a prescribed pressure or a prescribed flux condition that may or may not vary over time. Note that the prescribed pressure may need to be converted to a water head value depending on the code used.
9. Apply downstream drain boundary conditions in cells just above the water table to allow NAPL to drain out of the boundary at the downstream end above the water table.
10. With these modified parameters, apply the Richards Equation Solver towards simulation of LNAPL flow.
11. Translate the resulting LNAPL saturation which is in the modified porosity domain of equation (11) into the original porosity domain using equation (15).
12. Evaluate NAPL pressures and saturations, velocity vectors, mass balances from the solution to establish NAPL flow, storage, and other conditions of interest in zones within the model or within the entire model.

Example Problems

Two example problems are provided here to evaluate performance of the proposed simplifications by comparing the solution using a single phase flow equation with the multiphase solution using UTCHEM. The first example considers a flat bedding plane and a flat water table to note LNAPL migration through the unsaturated zone for various hydraulic conductivity and anisotropy values. The second example considers a sloping bedding plane and a sloping water table to note LNAPL migration for more complicated conditions. Simulation parameters for LNAPL (gasoline) and water used in these examples are noted on Table 1 unless specifically noted otherwise.

LNAPL migration through a horizontally bedded unsaturated soil to a horizontal water table

A simple example problem is presented to demonstrate the concepts that are discussed.

LNAPL migration through a sloping bedded unsaturated soil or along a sloping water table

Summary

A simplified approach has been presented for simulating migration of LNAPL in the vadose zone and on the water table. The approach greatly enhances robustness and efficiency for these evaluations as compared to performing multiphase flow simulations. Comparative examples demonstrate application and accuracy of the approach for evaluating LNAPL migration in environmental settings.

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Keywords

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